4,4'-Di-t-butylbiphenyl

Other names:	1,1'-biphenyl, 4,4'-bis(1,1-dimethylethyl)- 4,4'-bis(1,1-dimethylethyl)-1,1'-biphenyl 4,4'-di-tert-butyl-1,1'-biphenyl 4,4'-di-tert-butylbiphenyl DBB biphenyl, 4,4'-di-tert-butyl- p,p'-di-tert-butylbiphenyl
Inchi:	InChI=1S/C20H26/c1-19(2,3)17-11-7-15(8-12-17)16-9-13-18(14-10-16)20(4,5)6/h7-14H,1
InchiKey:	CDKCEZNPAYWORX-UHFFFAOYSA-N
Formula:	C20H26
SMILES:	CC(C)(C)c1ccc(-c2ccc(C(C)(C)C)cc2)cc1
Mol. weight [g/mol]:	266.43

Physical Properties

Property code	Value	Unit	Source
af	0.5313		Cheméo Relay (1.0)
hf	-24.55	kJ/mol	Cheméo Relay (1.0)
hfus	20.03	kJ/mol	Joback Method
hsub	106.80 ± 3.20	kJ/mol	NIST Webbook
hvap	86.20 ± 3.20	kJ/mol	NIST Webbook
ie	8.04	eV	Cheméo Relay (1.0)
log10ws	-7.65		Cheméo Relay (1.0)
logp	5.949		Crippen Method
mcvol	245.140	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
tb	614.83	K	Cheméo Relay (1.0)
tc	837.54	K	Cheméo Relay (1.0)
tf	400.80	K	Thermochemical studies of 4-tert-butylbiphenyl and 4,40-di-tert-butylbiphenyl
tf	392.00 ± 6.00	K	NIST Webbook
tf	390.00 ± 4.00	K	NIST Webbook
tf	402.00 ± 3.00	K	NIST Webbook
tf	395.00 ± 4.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.07	J/mol×K	713.86	Joback Method
cpg	712.81	J/mol×K	753.88	Joback Method
cpg	731.98	J/mol×K	793.89	Joback Method
cpg	749.69	J/mol×K	833.91	Joback Method
cpg	766.11	J/mol×K	873.92	Joback Method
cpg	781.38	J/mol×K	913.94	Joback Method
cpg	795.62	J/mol×K	953.95	Joback Method
dvisc	0.0005947	Pa×s	450.54	Joback Method
dvisc	0.0012913	Pa×s	397.88	Joback Method
dvisc	0.0003222	Pa×s	503.21	Joback Method
dvisc	0.0001960	Pa×s	555.87	Joback Method
dvisc	0.0001300	Pa×s	608.53	Joback Method
dvisc	0.0000920	Pa×s	661.20	Joback Method
dvisc	0.0000685	Pa×s	713.86	Joback Method
hfust	20.00	kJ/mol	400.80	NIST Webbook
hfust	18.80	kJ/mol	402.00	NIST Webbook
hvapt	108.63	kJ/mol	298.15	Vapour pressures and enthalpies of vaporization of a series of the alkylbiphenyls

Sources

Cheméo Relay (1.0):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1625918&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Cheméo Relay (1.0, beta):

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Thermochemical studies of 4-tert-butylbiphenyl and 4,4'-di-tert-butylbiphenyl: https://www.doi.org/10.1016/j.jct.2008.12.015

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Vapour pressures and enthalpies of vaporization of a series of the alkylbiphenyls: https://www.doi.org/10.1016/j.fluid.2012.08.020

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point